

4.0 Optimizing Workflow

Category: New User Orientation

This section provides additional basic tips on setting up your NAS environment to help make your workflow more efficient. Topics include use of the **module** command to select software versions, compiler commands, porting of MPI codes, and file management.

4.1 Setting up Your Environment

Setting up your environment to fit your needs makes it more convenient for you to use our systems.

4.1.1 Default Shell

When your account is created, your default shell is set to be **cs****h**; this is assumed to be the case throughout this guide.

If you want to use a different shell as your default, call the NAS Control Room at (800) 331-8737 or (650) 604-4444 or send an email message to support@nas.nasa.gov to request the change. Once the change is made, the new default shell of your choice applies to all of your NAS accounts on the various systems.

4.1.2 Module Commands

All NAS supercomputer systems use the **module** command to allow you to choose which versions of software packages--both licensed and freely available--to include in your own personal environment.

To use modules, be sure to include the following in your **.cshrc** file, which contains information that is read by the Linux shell (**cs****h** or **tcsh**) every time you log onto the computer or open a new terminal window:

```
source /usr/local/lib/global.cshrc
```

If you want to use modules for your current session only, use the following command:

```
% source /usr/share/modules/init/csh
```

The following are useful module commands to remember:

NAS Module Commands

<code>module avail</code>	find out what other modules are available
<code>module list</code>	list the modules in your environment
<code>module purge</code>	unload all loaded module files
<code>module load <i>module_name</i></code>	load new modules
<code>module switch <i>old_module_name</i> <i>new_module_name</i></code>	switch between different versions of software
<code>module show <i>module_name</i></code>	show changes to environment

4.1.3 Default Compilers and Software Modules

On Columbia, a default software set (including Intel compilers, SGI's Message Passing Toolkit, and SCSL libraries) is loaded automatically. Use the command `module list` to determine which modules have been loaded for you. If you prefer to use a non-default version, use the module commands in the table above to change to other versions in either your `.cshrc` file, your job script, or at the command line, depending on which sessions you want the change to take effect in.

On Pleiades, no default software is loaded. If you want to have a compiler, MPI library, math library, and so forth automatically loaded when you log in, use the `module load` command in your `.cshrc` or `.login` files. See also [Customizing Your Environment](#) for examples on how to set this.

4.2 Compiling Code with Intel Compilers

If you haven't used Intel compilers in the past, here are some commands to invoke the various versions:

```
ifort Intel Fortran
icc   Intel C
icpc Intel C++
```

For example, to compile `foo.f` with `ifort`, type:

```
% ifort foo.f
```

Read the `ifort`, `icc`, and `icpc` man pages for options to use. Type `man topic` to access the man page for a particular topic.

4.3 Porting and Running MPI Codes with SGI's MPT Library

To build an executable for your Message Passing Interface (MPI) code, we recommend taking the following steps:

- At the link step, link your code with SGI's MPT library by adding the option `-lmpi`
- Use the command `mpiexec` to start the MPI process

Note that on Pleiades, you need to first load an Intel compiler module and an SGI MPT module.

The example below shows how to compile and link your code with MPT:

```
% ifort -o foo foo.f -lmpi
```

For running your MPI codes with MPT in a PBS job, insert the following in your PBS script, where `xx` represents the number of MPI processes:

```
mpiexec -np xx foo
```

4.4 Managing Your Files

Quota Limits

Quota limits are enforced on all filesystems. Two kinds of quotas are supported:

- Limits on the total disk space occupied by a user's files
- Limits on how many files a user can store, irrespective of size; for quota purposes, directories count as files

Two types of quota limits are in place: hard limits and soft limits.

- Hard limits can never be exceeded-any attempt to use more than your hard limit will be refused with an error
- Soft limits can be exceeded temporarily
 - ◆ When you exceed your soft limit, you can continue to use your account on that system normally; however, you will receive a daily email message reminding you that you are over your soft quota limit, and you need to reduce your usage to below the soft limit
 - ◆ If you remain over your soft limit for more than the two-week grace period, the soft limit is enforced as a hard limit, and you will not be able to add or extend files or do any work (except removing files) until you get back under that limit

To check your disk usage and quota limits, use the command appropriate to the filesystem, as shown below:

Command	Filesystem
% <code>quota -v</code>	Columbia systems, Lou, and Pleiades home filesystems

```
% lfs quota -u your_nas_username  
/nobackup/your_nas_username
```

Pleiades /nobackup filesystems

4.5 Other Resources

You can get additional information such as user announcements, updates on technical issues, and advanced techniques related to the NAS supercomputing environment from the following links:

- [General User Information](#)
- [FAQ](#)
- [Knowledge Base Home](#)

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<http://www.nas.nasa.gov/hecc/support/kb/entry/265/?ajax=1>